Cyclohexane, 1,3,5-trimethyl-

Other names: 1,3,5-Trimethylcyclohexane
Inchi: InChI=1S/C9H18/c1-7-4-8(2)6-9(3)5-7/h7-9H,4-6H2,1-3H3
InchiKey: ODNRTOSCFYDTKF-UHFFFAOYSA-N
Formula: C9H18
SMILES: CC1CC(C)CC(C)C1
Mol. weight [g/mol]: 126.24
CAS: 1839-63-0

Physical Properties

Property code	Value	Unit	Source
gf	33.93	kJ/mol	Joback Method
hf	-215.45	kJ/mol	Joback Method
hfus	13.04	kJ/mol	Joback Method
hvap	35.44	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	3.079		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2648.83	kPa	Joback Method
rinpol	864.00		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	854.00		NIST Webbook
rinpol	864.00		NIST Webbook
rinpol	854.00		NIST Webbook
rinpol	853.00		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	851.00		NIST Webbook
tb	413.50 ± 2.00	K	NIST Webbook
tb	410.70 ± 1.00	K	NIST Webbook
tb	409.00 ± 4.00	K	NIST Webbook
tb	411.00 ± 3.00	K	NIST Webbook
tb	411.15 ± 2.00	K	NIST Webbook
tb	410.90 ± 2.00	K	NIST Webbook
tb	412.40 ± 2.00	K	NIST Webbook
tb	411.00 ± 4.00	K	NIST Webbook
tb	414.00 ± 3.00	K	NIST Webbook
tb	411.00 ± 3.00	K	NIST Webbook

tb	409.00 ± 5.00	K	NIST Webbook
tb	410.00 ± 5.00	K	NIST Webbook
tb	408.00 ± 4.00	K	NIST Webbook
tb	412.05 ± 1.00	K	NIST Webbook
tb	411.00 ± 6.00	K	NIST Webbook
tc	613.57	K	Joback Method
tf	190.09	K	Joback Method
vc	0.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.82	J/mol×K	415.53	Joback Method
cpg	273.92	J/mol×K	448.54	Joback Method
cpg	292.21	J/mol×K	481.54	Joback Method
cpg	309.72	J/mol×K	514.55	Joback Method
cpg	326.43	J/mol×K	547.56	Joback Method
cpg	342.37	J/mol×K	580.57	Joback Method
cpg	357.55	J/mol×K	613.57	Joback Method
dvisc	0.0024227	Pa×s	190.09	Joback Method
dvisc	0.0012236	Pa×s	227.66	Joback Method
dvisc	0.0007500	Pa×s	265.24	Joback Method
dvisc	0.0005190	Pa×s	302.81	Joback Method
dvisc	0.0003896	Pa×s	340.38	Joback Method
dvisc	0.0003096	Pa×s	377.96	Joback Method
dvisc	0.0002565	Pa×s	415.53	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1839630&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume